

Alexey T Zayak

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	A Ternary Map of Ni-Mn-Ga Heusler Alloys from Ab Initio Calculations. <i>Metals</i> , 2021, 11, 973.	1.0	4
2	Two Damping Mechanisms in the Chemically Enhanced Raman Scattering on Graphene: DFT Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24723-24730.	1.5	2
3	Ternary diagrams of magnetic properties of Ni-Mn-Ga Heusler alloys from ab initio and Monte Carlo studies. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 470, 64-68.	1.0	10
4	Peculiarities of phonons in Ni-Mn-Ga alloys: Ab initio studies. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 470, 73-76.	1.0	2
5	Empirical optimization of DFT+U and HSE for the band structure of ZnO. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 065501.	0.7	26
6	Glucose Sensing Using Surface-Enhanced Raman-Mode Constraining. <i>Analytical Chemistry</i> , 2018, 90, 14269-14278.	3.2	52
7	Ternary phase diagram of Ni-Mn-Ga: insights from ab initio calculations. <i>EPJ Web of Conferences</i> , 2018, 185, 05012.	0.1	1
8	Ab initio study of the composite phase diagram of Ni-Mn-Ga shape memory alloys. <i>Journal of Experimental and Theoretical Physics</i> , 2017, 125, 104-110.	0.2	5
9	Colloidal PbS Nanosheets with Tunable Energy Gaps. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1726, 13.	0.1	0
10	Compositional trends in Ni-Mn-Ga Heusler alloys: first-principles approach. <i>MATEC Web of Conferences</i> , 2015, 33, 05005.	0.1	4
11	Dehydrogenation of Ammonia on Ru(0001) by Electronic Excitations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10520-10525.	1.5	3
12	Raman Scattering from a Molecule-Semiconductor Interface Tuned by an Electric Field: Density Functional Theory Approach. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23113-23118.	1.5	16
13	Investigation of structural and magnetic properties of Heusler $\text{Fe}_{2+x}\text{Mn}_{1-x}\text{Al}$ alloys by first principles method. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2014, 11, 979-983.	0.8	3
14	Revealing Interaction of Organic Adsorbates with Semiconductor Surfaces Using Chemically Enhanced Raman. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 964-968.	2.1	12
15	Thickness-Controlled Synthesis of Colloidal PbS Nanosheets and Their Thickness-Dependent Energy Gaps. <i>Chemistry of Materials</i> , 2014, 26, 5433-5436.	3.2	73
16	Harnessing Chemical Raman Enhancement for Understanding Organic Adsorbate Binding on Metal Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1357-1362.	2.1	26
17	Transferable pair potentials for CdS and ZnS crystals. <i>Journal of Chemical Physics</i> , 2012, 136, 234111.	1.2	44
18	Chemical Raman Enhancement of Organic Adsorbates on Metal Surfaces. <i>Physical Review Letters</i> , 2011, 106, 083003.	2.9	123

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19	First-Principles Study of Confinement Effects on the Raman Spectra of Si Nanocrystals. Physical Review Letters, 2010, 105, 115504.	2.9	58
20	Lattice dynamics and structural stability of ordered $\text{Fe}_3\text{Mn}_3\text{O}_{10}$. Physical Review B, 2010, 81, .	1.1	45
21	Role of Confinement on Diffusion Barriers in Semiconductor Nanocrystals. Physical Review Letters, 2009, 102, 025901.	2.9	27
22	Pseudopotentials on Grids: Application to the Electronic, Optical, and Vibrational Properties of Silicon Nanocrystals. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1247-1261.	0.4	6
23	Algorithms for the electronic and vibrational properties of nanocrystals. Journal of Physics Condensed Matter, 2009, 21, 064207.	0.7	9
24	The phase diagram of $\text{Ni}_x\text{Mn}_y\text{Ga}$ alloys with account of crystal lattice modulation and external magnetic field. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 481-482, 218-222.	2.6	3
25	Magnetic-field-induced changes in magnetic shape memory alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 481-482, 258-261.	2.6	14
26	Influence of magnetism on the structural stability of cubic $\text{L}_{21}\text{Ni}_2\text{MnGa}$. European Physical Journal: Special Topics, 2008, 158, 193-198.	1.2	16
27	First-principles investigations of multimetallic transition metal clusters. Philosophical Magazine, 2008, 88, 2725-2738.	0.7	27
28	Manipulating magnetic properties of SrRuO_3 epitaxial and uniaxial strains. Physical Review B, 2008, 77, .	1.1	98
29	Minority-spin polarization and surface magnetic enhancement in Heusler clusters. Physical Review B, 2008, 77, .	1.1	15
30	Switchable $\text{Ni}_x\text{Mn}_y\text{Ga}$ Heusler nanocrystals. Journal of Applied Physics, 2008, 104, .	1.1	12
31	Ab initio modeling of martensitic transformations (MT) in magnetic shape memory alloys. Journal of Magnetism and Magnetic Materials, 2007, 310, 2761-2763.	1.0	9
32	Phase transitions in $\text{Ni}_x\text{Mn}_y\text{Ga}$ alloys with the account of crystal lattice modulation. Journal of Magnetism and Magnetic Materials, 2007, 316, e591-e594.	1.0	12
33	First-principles study of lattice instabilities in ferromagnetic $\text{L}_{12}\text{Fe}_3\text{Ni}$: direct force constants method versus linear response. Phase Transitions, 2006, 79, 853-861.	0.6	4
34	Structural, electronic, and magnetic properties of SrRuO_3 under epitaxial strain. Physical Review B, 2006, 74, .	1.1	162
35	ϵ -dependence of the lattice instability of cubic Heusler alloys from first principles. Applied Physics Letters, 2006, 88, 111903.	1.5	78
36	Modelling the phase diagram of magnetic shape memory Heusler alloys. Journal Physics D: Applied Physics, 2006, 39, 865-889.	1.3	306

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37	A critical discussion of calculated modulated structures, Fermi surface nesting and phonon softening in magnetic shape memory alloys Ni ₂ Mn(Ga, Ge, Al) and Co ₂ Mn(Ga, Ge). Journal of Magnetism and Magnetic Materials, 2005, 290-291, 874-877.	1.0	32
38	Ab initio calculations of the ferromagnetic shape memory alloy Ni _{1-x} Mn _x Al. Phase Transitions, 2005, 78, 267-276.	0.6	3
39	Ab initio study of the structure and dynamical properties of crystalline ice. Phase Transitions, 2005, 78, 179-196.	0.6	6
40	Atomic vibrational density of states of crystalline and amorphous FeSi ₂ thin films. Physical Review B, 2005, 71, .	1.1	21
41	Crystal structures of Ni ₂ MnGa from density functional calculations. Phase Transitions, 2005, 78, 259-266.	0.6	22
42	Anomalous vibrational effects in nonmagnetic and magnetic Heusler alloys. Physical Review B, 2005, 72, .	1.1	132
43	Magnetically driven shape memory alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 378, 52-60.	2.6	90
44	Role of shuffles and atomic disorder in Ni _{1-x} Mn _x Ga. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 378, 419-423.	2.6	42
45	Ab initio calculations of structure and lattice dynamics in Ni _{1-x} Mn _x Al shape memory alloys. Physical Review B, 2004, 70, .	1.1	55
46	First-principles investigations of homogeneous lattice-distortive strain and shuffles in Ni ₂ MnGa. Journal of Physics Condensed Matter, 2003, 15, 159-164.	0.7	80
47	First-principles investigation of phonon softenings and lattice instabilities in the shape-memory system Ni ₂ MnGa. Physical Review B, 2003, 68, .	1.1	109
48	A first-principles investigation of tetragonal and orthorhombic deformations in the ferromagnetic Heusler alloy Ni ₂ MnGa. European Physical Journal Special Topics, 2003, 112, 985-988.	0.2	14
49	A Ginzburg-Landau Theory For Ni-Mn-Ga. Phase Transitions, 2002, 75, 243-256.	0.6	20
50	Magnetoelastic influence on structural phase transitions in cubic ferromagnets. Journal of Magnetism and Magnetic Materials, 2002, 242-245, 1457-1459.	1.0	5
51	Phase transitions in ferromagnetic Ni _{2+x} Mn _{1-x} Ga alloys with regard for the modulation order parameter. Journal of Experimental and Theoretical Physics, 2001, 92, 1010-1018.	0.2	6
52	The influence of magnetoelastic interaction on structural phase transitions in cubic ferromagnets. Journal of Experimental and Theoretical Physics, 2001, 92, 1019-1023.	0.2	4
53	Structural phase transitions in cubic ferromagnets. Journal of Magnetism and Magnetic Materials, 1999, 191, 203-206.	1.0	10
54	Shape Memory Alloys: A Summary of Recent Achievements. Materials Science Forum, 0, 583, 21-41.	0.3	64

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55	Ternary Diagrams of Ni-Mn-Ga from First Principles. Materials Science Forum, 0, 845, 130-133.	0.3	1
56	Synthesis and Optical Spectroscopy of Colloidal PbS Nanosheets. , 0, , .		0
57	Synthesis and Optical Spectroscopy of Colloidal PbS Nanosheets. , 0, , .		0